Subgrain Size-Distributions, Dislocation Structures, Stacking- and Twin Faults and Vacancy Concentrations in Crystalline Materials Determined by X-ray Line Profile Analysis

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X-ray diffraction patterns, especially when measured with high precision, are a detailed fingerprint of the microstructure of crystalline materials. Up to date computer assisted numerical methods enable to describe whole diffraction patterns by physically well established profile functions based on specific microstructural models. Size profiles are modelled by assuming log-normal size-distribution of grains of subgrains. Distortion or strain profiles are base on the dislocation model developed by Wilkens. Stacking- and twin faults are incorporated by the method developed by Treacy et al. and are parametrized for the density of intrinsic-, extrinsic and twin faults, respectively. The diffuse background scattering is interpreted in terms of point defects, especially vacancies. It is shown that subgrains can be separated either (i) by tilt- or twist angles produced by geometrically necessary dislocations, or (ii) by dipolar dislocation walls whith no tilt or twist between the adjacent subgrains. Both types of subgrain boundaries break down the coherent scattering of X-rays, thus delineate undestorted crystalline regions in terms of X-ray scattering. Stacking- and twin faults are analysed in terms of splitting of dislocations, and are discussed as a function of grain- or subgrain size. Diffuse background scattering or background scattering, which is usually discarded as a disturbing part of diffraction patterns, is discussed in terms of vacancy concentrations within the grain interior and grain boundary regions, respectively. In plastically deformed copper it is shown that, when the deformation and the diffraction measurements are carried out at temperatures lower than the annealing temperatures of vacancies, relatively large vacancy concentrations, of the order of 10^{-7} - 10^{-6} are accumulating within the grain interior regions. More surprisingly, it is found that, within the grain-boundary or subgrain-boundary regions the vacancy concentration values can reach values corresponding to the metling remperature of copper, i.e. $5x10^{-5}$ - 10^{-4}. The microstructural parameters provided by X-ray line profile analysis will be discussed in specific case studies.

Keywords: microstructure, line profile analysis, subgrain size-distribution dislocations